```
data_lach41

_publ_section_comment
;
The two RPO groups C6H5PO and C3H5PO are disordered between the three
sites on the cluster, and also
disordered by symmetry.
Squeeze was carried out on the structural solution to allow for the
disordered solvent in the cell.
;

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
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;
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_chemical_melting_point           ?
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 'C63 H123 N3 O37 P3 Si W9'
_chemical_formula_weight          3290.29

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 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0311   0.0180
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0492   0.0322
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.2541   0.3302
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'W'  'W'  -5.4734   5.5774
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'P'  'P'   0.2955   0.4335
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            Trigonal
_symmetry_space_group_name_H-M    'R 3 m'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-y, x-y, z'
 '-x+y, -x, z'
 '-x+y, y, z'
 'x, x-y, z'
 '-y, -x, z'
 'x+2/3, y+1/3, z+1/3'
 '-y+2/3, x-y+1/3, z+1/3'
 '-x+y+2/3, -x+1/3, z+1/3'
 '-x+y+2/3, y+1/3, z+1/3'
 'x+2/3, x-y+1/3, z+1/3'
 '-y+2/3, -x+1/3, z+1/3'
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 '-x+y+1/3, y+2/3, z+2/3'
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 'x+1/3, x-y+2/3, z+2/3'
 '-y+1/3, -x+2/3, z+2/3'

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_cell_length_c                    18.889(3)
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_cell_angle_beta                  90.00
_cell_angle_gamma                 120.00
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_exptl_absorpt_correction_T_max   0.4585
_exptl_absorpt_process_details    'Sadabs'

_exptl_special_details
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;

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_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker Smart 6000 CCD'
_diffrn_measurement_method        'CCD scans'
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_diffrn_standards_interval_count  ?
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_diffrn_standards_decay_%         ?
_diffrn_reflns_number             13853
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_diffrn_reflns_av_sigmaI/netI     0.0644
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_diffrn_reflns_limit_k_max        23
_diffrn_reflns_limit_l_min        -20
_diffrn_reflns_limit_l_max        17
_diffrn_reflns_theta_min          3.28
_diffrn_reflns_theta_max          55.62
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_reflns_number_gt                 1700
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        SMART
_computing_cell_refinement        SAINTPLUS
_computing_data_reduction         SAINTPLUS
```

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_computing_structure_solution     SHELXTL
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0665P)^2^+0.0000P] where P=(Fo^2^+2Fc^2
^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details
 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    0.01(4)
_refine_ls_number_reflns          2390
_refine_ls_number_parameters      152
_refine_ls_number_restraints      66
_refine_ls_R_factor_all           0.0749
_refine_ls_R_factor_gt            0.0481
_refine_ls_wR_factor_ref          0.1141
_refine_ls_wR_factor_gt           0.1066
_refine_ls_goodness_of_fit_ref    0.967
_refine_ls_restrained_S_all       0.966
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 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
C1 C 0.733(2) 0.8664(10) 0.167(3) 0.105(17) Uiso 0.67(5) 2 d SPGU A 1
C2 C 0.676(3) 0.859(3) 0.129(3) 0.200 Uiso 0.33(3) 1 d PGU A 1
H2 H 0.6825 0.8796 0.0844 0.240 Uiso 0.33(3) 1 calc PR A 1
C3 C 0.609(3) 0.823(5) 0.158(4) 0.53(13) Uiso 0.33(3) 1 d PGU A 1
H3 H 0.5711 0.8176 0.1319 0.631 Uiso 0.33(3) 1 calc PR A 1
```

C4 C 0.599(2) 0.793(5) 0.224(3) 0.18(3) Uiso 0.33(3) 1 d PGU A 1
H4 H 0.5547 0.7680 0.2435 0.218 Uiso 0.33(3) 1 calc PR A 1
C5 C 0.656(3) 0.800(4) 0.263(2) 0.25(6) Uiso 0.33(3) 1 d PGU A 1
H5 H 0.6496 0.7801 0.3075 0.296 Uiso 0.33(3) 1 calc PR A 1
C6 C 0.723(2) 0.837(2) 0.234(3) 0.19(4) Uiso 0.33(3) 1 d PGU A 1
H6 H 0.7609 0.8421 0.2600 0.231 Uiso 0.33(3) 1 calc PR A 1
C1A C 0.762(6) 0.881(3) 0.199(6) 0.244(11) Uiso 0.33(5) 2 d SPDU A 2
H1A1 H 0.7646 0.8463 0.2281 0.293 Uiso 0.17(3) 1 calc PR A 2
H1A2 H 0.7646 0.9182 0.2281 0.293 Uiso 0.17(3) 1 calc PR A 2
C2A C 0.699(10) 0.849(5) 0.150(11) 0.244(10) Uiso 0.33(5) 2 d SPDU A
2
H2A H 0.6726 0.8033 0.1346 0.292 Uiso 0.17(3) 1 calc PR A 2
C7 C 0.690(11) 0.897(8) 0.135(12) 0.246 Uiso 0.17(3) 1 d PDU A 2
H7A H 0.7195 0.9408 0.1535 0.295 Uiso 0.17(3) 1 calc PR A 2
H7B H 0.6536 0.8896 0.1052 0.295 Uiso 0.17(3) 1 calc PR A 2
C8 C 0.618(3) 0.8089(14) 0.803(2) 0.23(2) Uiso 1 2 d SDU . .
H8A H 0.5937 0.7617 0.7848 0.270 Uiso 0.50 1 calc PR . .
H8B H 0.5937 0.8320 0.7848 0.270 Uiso 0.50 1 calc PR . .
C9 C 0.606(4) 0.8031(19) 0.886(2) 0.29(4) Uiso 1 2 d SDU . .
H9A H 0.6312 0.7806 0.9036 0.346 Uiso 0.50 1 calc PR . .
H9B H 0.6312 0.8506 0.9036 0.346 Uiso 0.50 1 calc PR . .
C10 C 0.536(3) 0.7682(17) 0.925(4) 0.47(5) Uiso 1 2 d SDU . .
H10A H 0.5098 0.7904 0.9116 0.561 Uiso 0.50 1 calc PR . .
H10B H 0.5098 0.7193 0.9116 0.561 Uiso 0.50 1 calc PR . .
C11 C 0.551(5) 0.775(2) 1.003(3) 0.47(5) Uiso 1 2 d SDU . .
H11A H 0.5072 0.7557 1.0285 0.708 Uiso 1 2 calc SR . .
H11B H 0.5788 0.8237 1.0153 0.708 Uiso 0.50 1 calc PR . .
H11C H 0.5746 0.7509 1.0161 0.708 Uiso 0.50 1 calc PR . .
C12 C 0.733(2) 0.8082(19) 0.795(2) 0.245(18) Uiso 1 1 d DU . .
H12A H 0.7776 0.8295 0.7710 0.294 Uiso 1 1 calc R . .
H12B H 0.7425 0.8168 0.8455 0.294 Uiso 1 1 calc R . .
C13 C 0.696(2) 0.7294(19) 0.783(2) 0.29(2) Uiso 1 1 d DU . .
H13A H 0.6789 0.7056 0.8276 0.342 Uiso 1 1 calc R . .
H13B H 0.6563 0.7160 0.7520 0.342 Uiso 1 1 calc R . .
C14 C 0.743(3) 0.707(2) 0.750(3) 0.39(4) Uiso 1 1 d DU . .
H14A H 0.7874 0.7282 0.7742 0.470 Uiso 1 1 calc R . .
H14B H 0.7503 0.7193 0.7006 0.470 Uiso 1 1 calc R . .
C15 C 0.705(3) 0.626(2) 0.759(3) 0.37(3) Uiso 1 1 d DU . .
H15A H 0.7363 0.6128 0.7784 0.562 Uiso 1 1 calc R . .
H15B H 0.6884 0.6044 0.7137 0.562 Uiso 1 1 calc R . .
H15C H 0.6656 0.6115 0.7904 0.562 Uiso 1 1 calc R . .
C16 C 0.683(2) 0.8414(10) 0.6911(18) 0.21(2) Uiso 1 2 d SDU . .
H16A H 0.6562 0.8635 0.6775 0.251 Uiso 0.50 1 calc PR . .
H16B H 0.6562 0.7927 0.6775 0.251 Uiso 0.50 1 calc PR . .
C17 C 0.751(2) 0.8754(11) 0.651(2) 0.25(2) Uiso 1 2 d SDU . .
H17A H 0.7779 0.8534 0.6632 0.298 Uiso 0.50 1 calc PR . .
H17B H 0.7779 0.9245 0.6632 0.298 Uiso 0.50 1 calc PR . .
C18 C 0.733(3) 0.8665(15) 0.572(2) 0.400 Uiso 1 2 d SDU . .
H18A H 0.7059 0.8885 0.5603 0.480 Uiso 0.50 1 calc PR . .
H18B H 0.7059 0.8174 0.5603 0.480 Uiso 0.50 1 calc PR . .
C19 C 0.803(4) 0.9017(18) 0.532(3) 0.400 Uiso 1 2 d SDU . .
H19A H 0.7950 0.9031 0.4825 0.600 Uiso 0.50 1 calc PR . .
H19B H 0.8266 0.8754 0.5396 0.600 Uiso 0.50 1 calc PR . .
H19C H 0.8321 0.9483 0.5495 0.600 Uiso 0.50 1 calc PR . .
N1 N 0.692(2) 0.8460(11) 0.7702(18) 0.218(17) Uiso 1 2 d SDU . .
O1 O 0.7917(8) 0.8958(4) -0.0347(10) 0.086(4) Uani 1 2 d SU . .
O2 O 0.7750(6) 0.7648(6) -0.0275(8) 0.105(4) Uani 1 1 d U . .
O3 O 0.9153(4) 0.8306(8) 0.0046(9) 0.084(4) Uani 1 2 d SU . .
O4 O 0.9180(7) 0.9590(4) 0.0006(8) 0.067(3) Uani 1 2 d SU . .
O5 O 0.8259(7) 0.8564(7) 0.0841(8) 0.105(3) Uani 1 1 d U A .
O6 O 0.8756(6) 0.8655(5) -0.1103(7) 0.078(3) Uani 1 1 d U . .
O7 O 1.0000 1.0000 -0.1133(13) 0.056(4) Uani 1 6 d SU . .
O8 O 0.9192(8) 0.9596(4) -0.2170(8) 0.077(4) Uani 1 2 d SU . .
O9 O 0.9198(5) 0.8397(10) -0.2376(9) 0.111(6) Uani 1 2 d SU . .
O10 O 0.8764(16) 0.9382(8) 0.1842(19) 0.184(11) Uani 1 2 d SU A .
Si1 Si 1.0000 1.0000 -0.0222(5) 0.0330(19) Uani 1 6 d SU . .

```
W1 W 0.84165(4) 0.84749(4) -0.01781(5) 0.0811(4) Uani 1 1 d U . .
W2 W 0.94994(3) 0.89987(6) -0.17865(6) 0.0740(4) Uani 1 2 d SU . .
P1 P 0.8209(5) 0.9105(2) 0.1327(5) 0.116(3) Uani 1 2 d SDU . .

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O1 0.051(8) 0.076(5) 0.123(12) 0.003(4) 0.005(8) 0.026(4)
O2 0.082(7) 0.062(6) 0.153(10) 0.023(6) 0.004(7) 0.022(5)
O3 0.078(5) 0.046(8) 0.116(12) 0.033(9) 0.016(5) 0.023(4)
O4 0.051(6) 0.056(5) 0.093(10) 0.007(3) 0.014(6) 0.026(3)
O5 0.095(9) 0.090(8) 0.130(6) 0.040(5) 0.034(6) 0.048(7)
O6 0.052(6) 0.062(6) 0.107(6) -0.010(5) -0.015(5) 0.018(5)
O7 0.059(6) 0.059(6) 0.052(8) 0.000 0.000 0.029(3)
O8 0.067(10) 0.097(6) 0.058(10) -0.010(4) -0.021(7) 0.034(5)
O9 0.136(12) 0.096(11) 0.089(11) -0.026(9) -0.013(4) 0.048(6)
O10 0.17(2) 0.138(15) 0.25(3) -0.033(9) -0.066(19) 0.087(12)
Si1 0.035(3) 0.035(3) 0.030(5) 0.000 0.000 0.0173(13)
W1 0.0575(5) 0.0582(5) 0.1160(8) 0.0132(5) 0.0139(5) 0.0202(4)
W2 0.0708(6) 0.0667(8) 0.0833(9) -0.0159(7) -0.0079(3) 0.0334(4)
P1 0.102(6) 0.115(5) 0.125(7) 0.021(3) 0.042(5) 0.051(3)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

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C1 C6 1.386(10) . ?
C1 P1 1.81(4) . ?
C2 C3 1.3900 . ?
C2 H2 0.9300 . ?
C3 C4 1.390(4) . ?
C3 H3 0.9300 . ?
C4 C5 1.390(2) . ?
C4 H4 0.9300 . ?
C5 C6 1.3900 . ?
C5 H5 0.9300 . ?
C6 H6 0.9300 . ?
C1A C2A 1.53(10) . ?
C1A P1 1.69(5) . ?
C1A H1A1 0.9700 . ?
C1A H1A2 0.9700 . ?
C2A C7 1.19(9) . ?
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C2A P1 2.4(2) . ?
C2A H2A 0.9300 . ?
C7 H7A 0.9300 . ?
C7 H7B 0.9300 . ?
C8 N1 1.55(5) . ?
C8 C9 1.58(3) . ?
C8 H8A 0.9700 . ?
C8 H8B 0.9700 . ?
C9 C10 1.52(3) . ?
C9 H9A 0.9700 . ?
C9 H9B 0.9700 . ?
C10 C11 1.51(3) . ?
C10 H10A 0.9700 . ?
C10 H10B 0.9700 . ?
C11 H11A 0.9600 . ?
C11 H11B 0.9600 . ?
C11 H11C 0.9600 . ?
C12 C13 1.53(3) . ?
C12 N1 1.58(4) . ?
C12 H12A 0.9700 . ?
C12 H12B 0.9700 . ?
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C13 H13A 0.9700 . ?
C13 H13B 0.9700 . ?
C14 C15 1.55(3) . ?
C14 H14A 0.9700 . ?
C14 H14B 0.9700 . ?
C15 H15A 0.9600 . ?
C15 H15B 0.9600 . ?
C15 H15C 0.9600 . ?
C16 N1 1.50(2) . ?
C16 C17 1.50(3) . ?
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C16 H16B 0.9700 . ?
C17 C18 1.53(3) . ?
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C17 H17B 0.9700 . ?
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C18 H18A 0.9700 . ?
C18 H18B 0.9700 . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
N1 C12 1.58(4) 5_565 ?
O1 W1 1.912(8) . ?
O1 W1 1.912(8) 5_565 ?
O2 W1 1.692(11) . ?
O3 W1 1.894(4) 4_655 ?
O3 W1 1.894(4) . ?
O4 Si1 1.629(14) . ?
O4 W1 2.214(10) . ?
O4 W1 2.214(10) 5_565 ?
O5 P1 1.555(15) . ?
O5 W1 1.984(15) . ?
O6 W1 1.865(14) . ?
O6 W2 1.923(13) . ?
O7 Si1 1.72(3) . ?
O7 W2 2.282(13) . ?
O7 W2 2.282(13) 3_675 ?
O7 W2 2.282(13) 2_765 ?
O8 W2 1.907(7) 3_675 ?
O8 W2 1.907(7) . ?
O9 W2 1.603(17) . ?
O10 P1 1.44(3) . ?
Si1 O4 1.629(14) 3_675 ?
Si1 O4 1.629(14) 2_765 ?
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W2 O6 1.923(13) 4_655 ?
P1 O5 1.555(15) 5_565 ?

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C2 C1 P1 123(3) . . ?
C6 C1 P1 117(3) . . ?
C3 C2 C1 119.9(3) . . ?
C3 C2 H2 120.0 . . ?
C1 C2 H2 120.0 . . ?
C2 C3 C4 120.0 . . ?
C2 C3 H3 120.0 . . ?
C4 C3 H3 120.0 . . ?
C5 C4 C3 120.00(15) . . ?
C5 C4 H4 120.0 . . ?
C3 C4 H4 120.0 . . ?
C4 C5 C6 120.00(14) . . ?
C4 C5 H5 120.0 . . ?
C6 C5 H5 120.0 . . ?
C5 C6 C1 120.06(14) . . ?
C5 C6 H6 120.0 . . ?
C1 C6 H6 120.0 . . ?
C2A C1A P1 95(10) . . ?
C2A C1A H1A1 112.8 . . ?
P1 C1A H1A1 112.8 . . ?
C2A C1A H1A2 112.8 . . ?
P1 C1A H1A2 112.8 . . ?
H1A1 C1A H1A2 110.2 . . ?
C7 C2A C1A 105(10) . . ?
C7 C2A P1 96(10) . . ?
C1A C2A P1 45(6) . . ?
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C1A C2A H2A 127.7 . . ?
P1 C2A H2A 119.2 . . ?
C2A C7 H7A 120.0 . . ?
C2A C7 H7B 120.0 . . ?
H7A C7 H7B 120.0 . . ?
N1 C8 C9 122(5) . . ?
N1 C8 H8A 106.9 . . ?
C9 C8 H8A 106.9 . . ?
N1 C8 H8B 106.9 . . ?
C9 C8 H8B 106.9 . . ?
H8A C8 H8B 106.7 . . ?
C10 C9 C8 127(6) . . ?
C10 C9 H9A 105.6 . . ?
C8 C9 H9A 105.6 . . ?
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